

Standard Form 298 (Rev. 2-89)
Prescribed by ANSI Std. Z39-18
298-102

OFFICE OF NAVAL RESEARCH GRANT N00014-89-J-3093

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FINAL PROGRESS REPORT

Annotated Bibliography of Published Papers Acknowledging Support of the Grant

1. Coherent Propagation of Waves in Intrinsically Nonuniform Media, Gabriel Cwlich and Yaotian Fu, *Physical Review B* **43**, 10448 (1991).

The authors develop a theoretical framework in which to study coherent propagation of waves in a random medium. Although most work in this field has been on random media that are statistically (on the average) uniform, this formalism allows for media that have fluctuations about a nonuniform average. This allows it to be used in describing media characterized by stratification as well as statistical fluctuations. Possible applications include acoustic waves in the ocean where the situation is complicated by variations and rapid fluctuations in temperature, pressure, and salinity of the water. All of these affect the sound velocity.

The authors show that the coherent effects are preserved in such a medium and can be treated by an extension of the uniform random medium formalism. In such a medium there are two length scales which characterize the medium; l and L which represent the distance that a wave travels before an appreciable change in its momentum takes place and the distance over which diffusive propagation takes place. This paper assumes that l is much less than L and that the wavelength of the medium is small compared to l .

Besides the development of the formalism, a study of the problem of backscattering in a stratified medium is studied in detail.

2. Scattering Delay and Renormalization of the Wave-Diffusion Constant, Gabriel Cwlich and Yaotian Fu, *Physical Review B* **46**, 12012 (1992).

This work extends the work of van Albada, van Tiggelen, Lagendijk, and Tip on the existence of a significant correction to the wave-diffusion constant. The authors give a very simple physical picture for the correction as a derivation for the case with weak disorder.

For classical waves in a random medium, the wave propagates as expected on a short length scale but diffusion takes place on a longer length scale because of disorder scattering. One can naively calculate the diffusion constant D by elementary transport theory using the mean free path. The explanation of the correction is that the scattering of a wave packet takes a finite time and this alters the diffusion constant. The correction is thus of a dynamical origin. Although the correction is usually small, this is not necessarily the case.

3. Atomistic Origins of Light-Induced Defects in a-Si, P. A. Fedders, Y. Fu, and D. A. Drabold, *Physical Review Letters* **68**, 1888 (1992).

This work presents an atomistic model of the formation of light induced defects in amorphous silicon. The formation of light induced defects is arguably the most important technological and scientific question today relating to a-Si. These defects cause a significant

reduction in the performance of a-Si photovoltaic devices. There have been many other models but none of them was based on detailed calculations or simulations. In this work the authors are mainly concerned with the microscopic origins of the effect rather than the kinetics on a more macroscopic scale.

Our model is based in part on our observations of molecular-dynamics simulations with an ab initio code and required a change in the charge of a well-localized state in the gap, such as a dangling bond, to nucleate the effect. The induced defects are then formed at weak bond sites in the network following a rearrangement caused by the change of the charge of the localized state. Our results indicate that the effect is nucleated by a localized defects state (such as a dangling bond) and that it is also necessary to have a strained volume of the material nearby. The weak bonds in the defect regions can then be broken by the change in charge of the defect state.

4. Second Virial Coefficient of an Interacting Anyon Gas, Daniel Loss and Yaotian Fu, *Physical Review Letters* **67**, 294 (1991).

In this paper the authors investigate the statistical mechanics of an interacting anyon gas with a repulsive pair potential of the form g/r^2 . The second virial coefficient is calculated and analyzed.

Anyons are particles obeying fractional statistics, and are controlled by a statistical parameter usually denoted by a , which can vary continuously. Interestingly enough, the limits of Fermi and Bose statistics can be studied as limiting cases. Anyon theory is of substantial interest to particle physicists.

It is shown that the second virial coefficient is a smooth function of a for negative values of g without cusps at the Bose point as it is for the non-interacting gas. However a cusp does develop as g approaches 0 and the order of limits of a and g is crucial.

5. Tight Binding Calculations for the Environmental Dependence of the Dangling Bond g-factor in a-Si, Y. Fu and P. A. Fedders, *Solid State Communications* **84**, 799 (1992).

In this paper the authors calculate the environmental (strain) dependence of the electron spin resonance g tensor for amorphous Si using a tight binding model of a dangling bond with Bethe lattice back bonding.

Dangling bond defects (3-fold coordinated Si atoms) generally determine the electrical and photoelectric properties of hydrogenated amorphous Si and thus are very important. The intensity of the dangling bond ESR line can be used to measure the quality of the sample and the linewidth should yield useful information about the sample. The g-value of the spin resonance is determined by the electronic structure of the surrounding atoms and thus can it can be used to investigate the structure around a dangling bond. We obtain a good fit to experimental data assuming only a Gaussian distribution of bond angles with an rms deviation of about 9 degrees, which is the generally accepted value for bond angle distortions in a-Si. Thus this work shows that the linewidth is inhomogeneous in nature and cannot be made narrower by any reasonable means.

6. Intrinsic Nonlinear Conductance of Mesoscopic Conductors, Hingsing Tang and Yaotian Fu, *Physical Review Letters* **67**, 485 (1991).

In this paper the conductance of a mesoscopic conductor is shown to be a sensitive function of the dc voltage applied to the system. This complements earlier work that showed that the conductance G was a sensitive function of the magnetic field, Fermi energy, and impurity configurations.

Experiments have shown the existence of strong nonlinear effects on conductance but there was no quantitative theory to explain the results. The present work remedies this. In the low-temperature limit, changing the potential drop across the system by an amount on the order of the level spacings of the system is sufficient to change the conductance by e^2/h . Arguments are presented based on scattering theory to support the authors' conclusions. Further, the theory is in good agreement with the results of harmonic generation experiments.

7. Transient Response in Quantum Transport of Noninteracting Electrons in Nanostructures, Yaotian Fu and Anand Ramaswami, *Physical Review B* **44**, 1088 (1991).

This paper discusses the evolution of the wave function of a system of noninteracting electrons in a nanostructure following a sudden change in the potential. It also points out that the transient evolution is not exponential in general. This is in contradiction to many assumed models.

The paper also contains an exact solution for a model system to support the work. It is suggested that the dephasing time is the relevant time for an exponential transient.

8. Microwave response of Mesoscopic Rings, Hing Sing Tang and Yaotian Fu, *Physical Review B* **46**, 3854 (1992).

Mesoscopic systems are those small enough that the size is comparable or less than the mean free path for electrons. These systems have a number of interesting properties including a nonlocal contribution to the conductivity. Experimentally this has been shown to depend sensitively on the configuration of the entire sample.

In this paper the authors consider the scattering of microwave radiation by a mesoscopic ring in the high frequency limit where the frequency is comparable to the inverse of the diffusion time around the circuit. In this case the microwave scattering intensity acquires a nontrivial frequency dependence that is explored.

9. Quantum Inductance within Linear Response Theory, Yaotian Fu and Scott C. Dudley, *Physical Review Letters* **70**, 65 (1993).

The authors derive the Landauer-Buttiker formula for admittance from linear response theory. Much of the current understanding of dc quantum transport in mesoscopic systems is based on this formula which recognizes the wave nature of the transport process and relates the conductance to the quantum transmission and reflection amplitudes of the system. In this case the L-B theory is derived for ac response which is much more complex than the dc case.

Beside giving an important addition to theory, the result is applied to a system which displays a resonance and it is shown that the admittance has an inductive component proportional to the lifetime of the resonance.

10. Dephasing, dissipation, and persistent current in a mesoscopic normal metal ring, Changsoo Park and Yaotian Fu, *Physics Letters A* **161**, 381 (1992).

The persistent current in a normal (as opposed to superconducting) ring is a mesoscopic quantum phenomenon. Unlike superconductivity, mesoscopic quantum effects exist only in samples smaller than the dephasing length, defined roughly as the characteristic length scale over which the coherence of the wave function is preserved. This notion of dephasing is central to the study of mesoscopic physics and is distinct from inelastic scattering.

In the present work the authors theoretically study the persistent current in a normal mesoscopic metal ring using the model of an electron couples to an infinite set of harmonic oscillators. These oscillators act as the lattice vibrations in the metal. They find that for the case of ohmic dissipation, the quantum interference is suppressed and the persistent current is destroyed

11. Inhomogeneous particle-density distribution in a current-carrying mesoscopic conductor, Hing Sing Tang and Yaotian Fu, *Physical Review B* **46**, 12761 (1992).

The view that transport should be viewed as a wave transmission process in mesoscopic physics is now well accepted. Further, the internal electric field in a mesoscopic system is inhomogeneous, in contrast to regular conductors.

In this paper the authors study the residual resistivity dipole in a system with multiple coherent scattering. The particle density distribution is calculated and shown to have fluctuations with both short- and long-range correlations.